Manual Assignment of NMR data

[Too specific??

* 2 methods: those that require spin systems (group of coupled nuclei with cross-peaks in one or more spectra), those that don’t
* Without spin systems, the methods require:
  + high quality peak lists with few missing/false peaks
  + little difference in the chemical shift of the same nucleus in different spectra.
* With two main sections of data, one with fairly consistent data and the other with a lot of missing peaks, we would (if manually assigning) use the former of the methods.]

Chemical shifts of C(alpha) and C(beta) atoms used for preliminary identification of amino acid type

- C(a/b) chemical shifts adopt values characteristic of amino acid type

- need to compare data to find sequential connectivity from each amino acid to the preceding one.

In most cases, backbone NMR data is assigned manually. However, with hundreds of values for the chemical shift values of C(a) and C(b), this process can take anywhere from 20 days to 9 months with perfect data. To complicate matters even more, experience has shown most data sets to have missing or false peaks, requiring whomever is doing the actual assignment to either skip large portions of the protein sequence or to guess where a certain chain is located in the sequence, making this method extremely error prone.

---------- Get info from Dr. Kilpatrick about our data sets: Calmodulin------------